1N161611111 7N-43-CR

Semi-annual Report for January - June, 1996 Kendall L. Carder, University of South Florida NAS5-31716

Abstract

The algorithm-development activities at USF during the first six months of 1996 have concentrated on field data collection and theoretical modeling. One bio-optics experiment was conducted during an AVIRIS overflight in the Florida Keys area. One Gulf of Alaska/Bering Sea cruise accompanied by a NOAA P3 airplane overflight was completed. Two papers were published. Two papers were submitted for publishing. Two abstracts were submitted for a conference presentation.

Tasks Accomplished:

- 1. Remote sensing reflectance, global spectral irradiance from a Licor 1800, and Reagan sun-photometric data were collected during an AVIRIS overflight (March 23) campaign near the Florida Keys from March 12 March 26.
- 2. The Gulf of Alaska/Bering Sea expedition during April 17 to April 29 was completed. The research ship time and the P3 airplane overflight were funded by NOAA. The samples collected showed high level of pigment packaging effect. These are an excellent data set to evaluate high-latitude parameterization of chl a algorithm.
- 3. A paper titled "Estimating primary production at depth from remote sensing" by Lee at el. has been published in Applied Optics.

Using a common primary production model, and identical photosynthetic parameters, four different methods were used to calculate quanta (Q) and primary production (P) at depth for a

study of high-latitude, North Atlantic waters. The differences among the 4 methods relate to the use of pigment information in the upper water column. Methods 1 and 2 use pigment biomass (B) as an input, and a subtropical, empirical relationship between $K_d(\lambda)$ (diffuse attenuation coefficient) and B to estimate Q at depth. Method 1 uses measured B, but Method 2 uses CZCS-derived B (subtropical) as inputs. Methods 3 and 4 both use phytoplankton absorption spectra $(a_{\phi}(\lambda))$ data that were calculated remotely instead of B as input Method 3, however, use $a_{\phi}(\lambda)$ and $K_d(\lambda)$ values empirically derived from remote-sensing, while Method 4 use analytically derived $a_{\phi}(\lambda)$ and $a(\lambda)$ (total absorption coefficient) spectra based on hyperspectral remote measurements.

In comparing calculated to measured values of Q(z) and P(z), Method 4 provided the closest results $[P(z): r^2 = 0.95 \text{ (n = 24)};$ and $Q(z): r^2 = 0.92 \text{ (n = 11)}]$. Method 1 gave the worst results $[P(z): r^2 = 0.56;$ and $Q(z): r^2 = 0.81]$. These results indicate that the analytically derived $a_{\phi}(\lambda)$ and $a(\lambda)$ can be applied to accurately estimate P(z) based on ocean-color remote sensing. Curiously, application to subarctic waters of algorithms for B and K_d , both of which were empirically developed using subtropical and summer temperate data sets, apparently compensate to some extent for effects due to their implicit dependence on pigment-specific absorption coefficients (a_{ϕ}^*) . Clearly using incorrect specific absorption coefficients(subtropical) for both the B and K_d algorithm is better than using measured B(subarctic) with a subtropically "tuned" K_d algorithm (compare Methods 1 & 2). Since remote estimates of B depend on a_{ϕ}^* and a_{ϕ}^* varies temporally and spatially, a method independent of B was sought. By rearranging the CZCS algorithm and the primary production expressions, using a_{ϕ} instead of B as an input to the P expression, and relating the CZCS algorithm to a_{ϕ} instead of B, improved results for estimating P from remotely sensed data were derived for use with CZCS class sensors. Most importantly, there

is no dependence with this method on an accurate estimations of pigment-specific absorption coefficients (a_{ϕ}^{*}) for application of the absorption-based methods (Methods 3 and 4).

4. A paper titled "Method to derive ocean absorption coefficients from remote-sensing reflectance" by Lee at el. has been published in Applied Optics.

A method to analytically derive in-water absorption coefficients from total remote-sensing reflectance (ratio of the upwelling radiance to downwelling irradiance above the surface) is presented. For measurements made in the Gulf of Mexico and Monterey Bay, with concentrations of [$chl\ a$] ranging from 0.07 to 50 mg/m³, comparisons are made for the total absorption coefficients derived using the suggested method and those derived using diffuse attenuation coefficients. For these coastal to open ocean waters, including regions of upwelling and the Loop Current, the results are as follows: at 440 nm the root-mean-square difference between the two is 13.0% ($r^2 = 0.96$) for total absorption coefficients ranging from 0.02 to 2.0 m¹; at 488 nm the difference is 14.5% ($r^2 = 0.97$); and at 550 nm the difference is 13.6% ($r^2 = 0.96$). The results indicate that the method presented works very well for retrieving in-water absorption coefficients exclusively from remotely measured signals, and that this method has a wide range of potential applications in oceanic remote sensing. The absorption coefficient can be used to estimate the light field at depth and the absorption of photons by phytoplankton (e.g. Section 3).

5. Newly revised versions of chlorophyll a, IPAR, and clear water epsilon software packages have been delivered to the MODIS ocean team to be merged into the MODIS Beta delivery package. The computer code for the algorithm has changed slightly. The algorithm equations are now solved algebraically, rather than with a two-dimensional lookup table (see Figure 1). The new code also allows more flexibility in modification. The algorithm still produces the same results to within less than one percent, but it runs in about 70% of the time it

took the old code to run (see Speed Test section). More diagnostic output has alsobeen written into the code to better analyze it's performance.

The algorithm programs are now more integrated with the rest of the MODIS ocean color processing scheme. The code for the clear-water epsilon algorithm has been simplified substantially by incorporating it into Howard Gordon's atmospheric correction code. The code for the instantaneous photosynthetically available radiation/absorbed radiation by phytoplankton algorithm has been simplified.

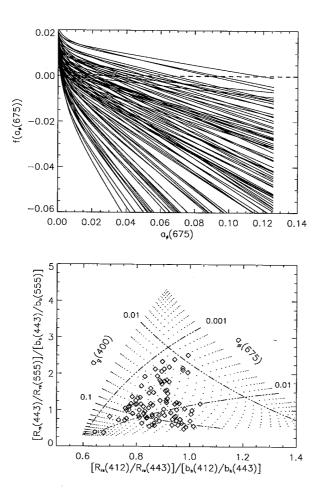


Figure 1.

The top panel illustrates the new algorithm solution. Each line, corresponding to one pixel of Rrs input, is a 33-element array representing an algebraic function of a_phi(675). a_phi(675) is determined by finding the zero of this function. Chloropyll concentration and a_g(400) are calculated from this value.

The bottom panel illustrates the old algorithm solution. Each diamond corresponds to one pixel of Rrs input and the matrix of dots represents the lookup table, a 33-by-33 array. The lookup table is searched until the input point is located within a block of four points and a_phi(675) and a_g(400) are then determined by interpolating between these points. Chlorophyll concentration is then calculated from the a_phi(675) value.

6. A paper titled "SeaWiFS Algorithm for Chlorophyll *a* and Colored Dissolved Organic Matter in Subtropical Environments" by Kendall L. Carder, Steven K. Hawes, and Zhongping Lee has been submitted to Applied Optics for publication.

Semi-analytical algorithms for phytoplankton and gelbstoff absorption and for chlorophyll a concentration are presented for use with the SeaWiFS sensor planned for launch on the SeaStar spacecraft in 1996. With slight modifications for spectral differences, the algorithms can be used with the Japanese Ocean Color and Temperature Scanner planned for launch by NASDA on the ADEOS satellite in 1996 and the Moderate Resolution Imaging Spectrometer planned for launch by NASA on EOS-1 in 1998. The approach is to separate absorption by gelbstoff and detritus from that by phytoplankton using the 412, 443, and 555 nm spectral bands. For waters with chlorophyll a concentrations of more than about 5 mg m⁻³, the algorithm saturates and switches to an empirical version relying on the 490-to-555 nm band ratio. In non-upwelling tropical and subtropical waters and summer temperate waters, the algorithm predicts phytoplankton absorption and chlorophyll a concentration with root-mean-square errors less than 32%. Waters tested are from the Arabian Sea, the North Pacific, the North Atlantic, and the Gulf of Mexico, with chlorophyll a concentrations ranging from 0.05 to 40 mg m⁻³. The algorithm underestimates chlorophyll a concentration by about a factor of two for spring bloom and upwelling sites, and a similar error is expected for high-latitude waters. Accuracies for such sites can be improved simply by using parameters for phytoplankton absorption characterization consistent with the site and season.

7. A paper titled "Pigment packaging and chlorophyll a-specific absorption in high-light oceanic waters" by Bissett at el. was revised and resubmitted to Limnology and Oceanography for publishing.

The absorption of light by particles at a single wavelength, $a_{\phi}(\lambda)$, is reduced with increased packaging of the light absorption material within these particles. This reduction can be described by the parameter Q^*a :

$$Q_a^*(\lambda) = \frac{a_{\phi}(\lambda)}{a_{sol}(\lambda)} = \frac{a_{\phi}(\lambda)}{S \cdot a_{om}(\lambda)}$$

where $a_{sol}(\lambda)$ is the theoretical maximum light absorption of the cellular material, a_{om} , in a completely dissolved state(solution). In practice, the estimations $a_{sol}(\lambda)$ for living phytoplankton are hampered by the process of removing the light absorptive material (pigments) from the organic matrix of the cell. The estimations of $a_{sol}(\lambda)$ can be further hampered by the destruction of the pigment-protein complexes when an organic solvent is used to strip the pigment from the cell. What is actually being measured by any of the current methods trying to determine $a_{sol}(\lambda)$ is $a_{om}(\lambda)$, i.e. the absorption of light by the pigment material in the organic medium of the experiment (methanol, acetone, Triton-X, etc.) The solvation factor, S, in the above equation is the ratio of the true $a_{sol}(\lambda)$ to the measured $a_{om}(\lambda)$.

We have developed an internally consistent measure of $a_{\phi}(\lambda)$, $a_{om}(\lambda)$, chlorophyll a concentration, and pheopigment concentration to determine the value of $Q^*a \cdot S$. This relationship is used to determine a functional relationship for chlorophyll a absorption for high-light-adapted, natural phytoplankton populations in optically clear waters. The packaging effect in these waters is negligible at the red end of the spectrum. Exclusion of the weight-specific absorption of pheopigments and the assumption of a zero $a_{\phi}(\lambda)$ at a zero pigment (chlorophyll a + pheopigment) concentration produces a misleading chlorophyll a-specific absorption and a false determination of pigment packaging. An algorithm is developed for predicting chlorophyll a

concentration from $a_{\phi}(675)$.

8. Significant progress has been made on development of a 3_D Monte Carlo radiative transfer model. It has been successfully tested on the 1-D model scenario set forth in Mobley et al. (1994) and is now being parameterized for use in evaluating land- and cloud-induced adjacency effects(e. g. see Reinersman & Carder) on ocean radiance retrievals. With good MTF estimates for large-swath instruments such as MODIS, SeaWiFS, and AVHRR, the separate contributions of land and clouds versus instrument stray light can be evaluated for various viewing scenarios.

This package of subroutines has been implemented which allows rapid development of Monte Carlo simulations of radiative transfer in fairly general three dimensional (3-d) environments. The source code was written in the C++ programming language, and is implemented in a straight-forward manner intended to be accessible to scientific (i.e. novice) programmers. The language provides the power of object oriented programming to build models of physical situations from basic geometric objects. The source code now in use has been extensively commented, and is robust against most common types of errors.

While the system is still under development, primary design concerns continue to be generality, expandability, and clarity. Meeting these goals requires some sacrifice; memory requirements are somewhat greater than problem-specific code would require, and execution speed is substantially reduced. But computer memory is becoming more plentiful, and personal computers (PC's) with over 100 megabytes of ram are becoming commonplace. The penalty of increased execution time is more than offset by the savings in time required to construct and validate the code for each new simulation.

A Monte Carlo simulation of the atmospheric point spread function was constructed to test the results of the system against previously published results. The earth surface and the 50

layers of Elterman's atmosphere were constructed with minimal effort using system subroutines, and are now filed for use in other simulations. For consistency, photon-tracing logic was implemented to duplicate the algorithm in the previous work. Because in the newer model the geometric work is performed by calls to class-member functions which have been tested previously for correctness, debugging involved no more than correction of a few programming mistakes. Preliminary analysis of the results of the simulation with the newer code indicate excellent agreement with the previous model.

Future work on this system will proceed on parallel paths. As new simulations require the construction of new physical objects or new optical processes, the new code will be archived for reuse. Then, as the library of code expands, development time for future simulations will be reduced.

Additionally, the geometric capabilities of the system must be enhanced. The system now has the capability to model objects bounded only by polyhedra. This restriction will be relieved by development of objects bounded by more general curved surfaces. These objects will require implementation of the geometric functions necessary to manipulate them.

Finally, as the system matures, a graphical user interface should be employed to further speed the construction of simulated scenes. The system now requires numerical input from the keyboard to construct objects which could be more conveniently constructed in the manner of typical computer assisted design (CAD) packages.

9. An abstract titled "Remote-sensing reflectance and inherent optical properties of oceanic waters derived from above-water measurements" By Lee at el. was submitted to the Ocean Optics XIII conference in Halifax, Nova Scotia, Canada, Oct. 22-25, 1996 for presentation.

Remote-sensing reflectance (Rrs, ratio of the water-leaving radiance to downwelling irradiance just above the surface) and inherent optical properties of oceanic waters are important. parameters for ocean optics. Due to skylight reflectance, Rrs or water-leaving radiance is difficult to measure from above the surface. It usually is derived by correcting for the reflected skylight in the measured above-water upwelling radiance. This correction can be erroneous, however, when the sea surface is not flat and the sky is not clear in the reflected field. We partition the skylight into Rayleigh and aerosol contributions, remove the Rayleigh contribution using the Fresnel reflectance, and correct the aerosol contribution using an optimization algorithm. During the procedure Rrs and in-water inherent optical properties are also derived. For measurements of 45 sites made in the Gulf of Mexico and Arabian sea with chlorophyll_a concentrations ranging from 0.07 to 50 mg/m³, the derived Rrs and inherent optical property values were compared with those from in-water measurements. It was found that the ratios of Rrs values at 440 and 550 nm were very consistent ($R^2 = 0.97$, 10.8% Root-Mean-Square-Difference for chl_a < 1 mg/m³). This type of ratio is used in pigment algorithm for satellite-derived data. For the derived inherent optical properties, the total absorption coefficients and particle absorption coefficients agreed well with their in-water values (16.2% and 19.0% RMSD, respectively). These results indicate that for the waters studied, the proposed procedure performs quite well in deriving Rrs and in-water inherent optical properties from above-water measurements.

10. A paper titiled "Polarization of remote-sensing reflectance measured 90° to the solar plane" by Lee, Z.P., Carder, K.L., Peacock, T.G., Steward, R.G., was submitted to the Ocean Optics XIII conference in Halifax, Nova Scotia, Canada, Oct. 22-25, 1996 for presentation.

Remote-sensing reflectance (ratio of the water-leaving radiance to the downwelling

plane and in a direction 30° to nadir. These measurements, carried out to see if the water-leaving, radiance in that direction is highly polarized, were made with and without a vertical polarizer in front of the sensor. For 28 pairs of measurements with chlorophyll_a concentrations ranging from 0.07 to 38 mg/m³, sun angles from 18° to 66° from zenith, clear to cloudy skies, and for optically shallow and deep waters, we did not see significant variations between the polarized and unpolarized results. Statistical comparisons of polarized to unpolarized results provided R² values of 0.990, 0.998, and 0.999 with slopes 1.011, 0.981 and 1.009 for wavelengths at 440, 550 and 630 nm, respectively. These results suggest that although the under water light field is partially polarized, the water-leaving radiance 90° to the solar plane and 30° (22° underwater) to the nadir is not highly polarized.

PUBLICATIONS

Carder, K.L., S. K. Hawes, and Z.P. Lee, SeaWiFS Algorithm for Chlorophyll *a* and Colored Dissolved Organic Matter in Subtropical Environments (submitted to J.G.R.).

Bissett, W.P., J. Patch, K.L. Carder, and Z.P. Lee. Pigment packaging and chlorophyll a-specific absorption in high-light oceanic waters (resubmitted to Limnology and Oceanography).

Lee, Z.P., K.L. Carder, J. Marra, R.G. Steward, M.J. Perry, 1996. Estimating primary production at depth from remote sensing, Applied Optics, 35(3):463-474.

Lee, Z.P., K.L. Carder, T.G. Peacock, C.O. Davis, and J.L. Mueller, 1996. Method to derive ocean absorption coefficients from remote sensing reflectance, Applied Optics, 35(3):453-462.

Lee, Z.P., K.L. Carder, Remote-sensing reflectance and inherent optical properties of oceanic waters derived from above-water measurements,. Ocean Optics XIII conference in Halifax, Nova Scotia, Canada, Oct. 22-25, 1996.

Lee, Z.P., K.L. Carder, Polarization of remote-sensing reflectance measured at 90 degrees to the solar plane, Ocean Optics XIII conference in Halifax, Nova Scotia, Canada, Oct. 22-25, 1996.

Anticipated Activities:

- 1. The relationships between temperature anomalies and the packaging effect and nutrients will be explored in order to reduce uncertainty in the chlorophyll algorithm Bering Sea data and upwelling data from Arabian Sea and Montery Bay will be used in the analyses.
- 2. Identifying AVIRIS images containing well defined clouds and shadows using machine learning methods(neural networks) before the images have been calibrated and corrected for atmospheric effects will be attempted.
- 3. Two papers are in preparation by Lee et al.: a. "Removal of reflected sky-light and retrieval of in-water inherent optical properties using water remote-sensing reflectance". And b. "Polarization of remote-sensing reflectance measured at 90 degrees to the solar plane".
 - 4. Research expeditions underway or to be completed:
 - a. Coastal Benthic Optical Properties (COBOP)
 - 1) July 10 July 24
 - 2) ONR-funded ship time and aircraft overflight time
 - 3) Three major transect lines in coral reef environment will be studied along with,

one deep water, oligotrophic station offshore used to calibrate airplane data.

4) Data set useful for developing bottom-discrimination algorithms and to observe error induced by bottom reflectance.

b. East China Sea

- 1) July 15 to August 5
- 2) Taiwan NSF-funded ship time
- 3) Transects from Kuroshio onto the continental shelf and into coastal plumes from rivers.
- 4) Test and modify Case II chl a algorithm for CDOM-rich waters.

c. Chesapeake Outflow

- 1) September 13 to 28
- 2) ONR-funded shiptime
- 3) Transects from the mouth of Chesapeake Bay to Cape Hatteras
- 4) Test and modify Case II chl a algorithms for CDOM-rich waters.

d. Gulf of Mexico/ Mississippi River

- 1) November 15 to 30 (scheduled)
- 2) MODIS-funded shiptime
- 3) Transects from the Loop Current into the Mississippi River plume and onto the West Florida Shelf.
- 4) Test/modify Case I and Case II MODIS algorithms using OCTS data for the first time.